Intermediate Quantum Mechanics
Lecture 7 Notes (2/11/15)
Position and Momentum Operators

The position operator, $\hat{x}$

- The position operator, $\hat{x}$, in the x-representation, multiplies $\psi(x)$ by x.

$$|\psi\rangle \xrightarrow{|x\rangle} \langle x\,|\,\psi\,\rangle = \psi(x)$$

$$\hat{x}\,|\psi\rangle \xrightarrow{|x\rangle} \langle x|\hat{x}\,|\psi\rangle = x\psi(x)$$

- Is $\hat{x}$ Hermitian? $\langle\phi|\hat{x}\,|\psi\rangle^* \stackrel{?}{=} \langle\psi|\hat{x}\,|\phi\rangle$

$$\langle\phi|\hat{x}\,|\psi\rangle^* = \left[\int \langle\phi\,|\,x'\,\rangle\langle x'|\hat{x}\,|\psi\rangle\,dx'\right]^* = \left[\int \phi^*(x')x'\psi(x')\,dx'\right]^*$$

$$= \int \phi(x')x'\psi^*(x')\,dx' = \int \psi^*(x')x'\phi(x')\,dx' = \langle\psi|\hat{x}\,|\phi\rangle$$

- The eigenfunctions of $\hat{x}$ are states of definite position, $|x_0\rangle$.

$$\langle x\,|\,x_0\,\rangle = \delta(x - x_0) = \psi_{x_0}(x)$$

The derivative operator, $\hat{D}$

- Next consider the derivative operator $\hat{D}$

$$\hat{D}\,|\psi\rangle \xrightarrow{|x\rangle} \langle x|\hat{D}\,|\psi\rangle = \frac{d}{dx}\,\psi(x)$$

- Is $\hat{D}$ Hermitian? $\langle\phi|\hat{D}\,|\psi\rangle^* \stackrel{?}{=} \langle\psi|\hat{D}\,|\phi\rangle$

$$\langle\phi|\hat{D}\,|\psi\rangle^* = \left[\int \langle\phi\,|\,x'\,\rangle\langle x'|\hat{D}\,|\psi\rangle\,dx'\right]^* = \left[\int \phi^*(x')\,\frac{d}{dx'}\,\psi(x')\,dx'\right]^*$$

Integrate this by parts.

$$\left[\int \phi^*(x')\,\frac{d}{dx'}\,\psi(x')\,dx'\right]^* = -\left[\int \left(\frac{d}{dx'}\,\phi^*(x')\right)\psi(x')\,dx'\right]^* + \left[\phi^*(x)\psi(x)\Big|_{-L/2}^{L/2}\right]^*$$

We require that the functions $\phi(x)$ and $\psi(x)$ go to zero at the end points. Then $\phi^*(x)\psi(x)\Big|_{-L/2}^{L/2} = 0$ and we then have.

$$\langle\phi|\hat{D}\,|\psi\rangle^* = -\left[\int \left(\frac{d}{dx'}\,\phi^*(x')\right)\psi(x')\,dx'\right]^* = -\int \psi^*(x')\,\frac{d}{dx'}\,\phi(x')\,dx' = -\langle\psi|\hat{D}\,|\phi\rangle$$

$\hat{D}$ is anti-Hermitian, $\hat{D}^\dagger = -\hat{D}$.

The k operator, $\hat{k}$

- It's easy to see how to make the derivative operator Hermitian. Multiply it by i or $-i$. $\hat{k} = -i\hat{D}$

$$\hat{k}\,|\psi\rangle \quad \xrightarrow{|x\rangle} \quad \langle x|\hat{k}\,|\psi\rangle \;=\; -i\,\frac{d}{dx}\,\psi(x)$$

- Let $|k_0\rangle$ be an eigenfunction of $\hat{k}$ with eigenvalue k_0.

$$\hat{k}\,|k_0\rangle \;=\; k_0\,|k_0\rangle \qquad\qquad \langle x|\hat{k}\,|k_0\rangle \;=\; k_0\,\langle x\,|\,k_0\,\rangle \;=\; k_0\psi_{k_0}(x)$$

But we also have: $\langle x|\hat{k}\,|k_0\rangle \;=\; -i\,\dfrac{d}{dx}\,\psi_{k_0}(x)$.

$$-i\,\frac{d}{dx}\,\psi_{k_0}(x) \;=\; k_0\psi_{k_0}(x) \qquad \Rightarrow \qquad \psi_{k_0}(x) \;=\; Ae^{ik_0x}$$

- Normalization of $|k_0\rangle$

$$\langle k\,|\,k_0\,\rangle \;=\; \int \langle k\,|\,x'\,\rangle\,\langle x'\,|\,k_0\,\rangle\,dx' \;=\; |A|^2 \int e^{-ikx'}e^{ik_0x}\,dx'$$

$$=\; |A|^2 \int e^{i(k_0-k)x'}\,dx' \;=\; |A|^2\,\delta(k-k_0)$$

We choose $A \;=\; \dfrac{1}{\sqrt{2\pi}}$ so that the eigenstates of $\hat{k}$ are normalized to the δ-function.

The k-representation

- Since $\hat{k}$ is a Hermitian operator, its eigenvectors form a complete basis.
- Just as we can expand $|\psi\rangle$ in terms of the $\hat{x}$ eigenfunctions:

$$|\psi\rangle \;=\; \int \psi(x')\,|x'\rangle\,dx' \qquad \text{where} \qquad \psi(x) \;=\; \langle x\,|\,\psi\,\rangle$$

we can alternatively expand $|\psi\rangle$ in terms of the $\hat{k}$ eigenfunctions:

$$|\psi\rangle \;=\; \int \tilde{\psi}(k')\,|k'\rangle\,dk' \qquad \text{where} \qquad \tilde{\psi}(k) \;=\; \langle k\,|\,\psi\,\rangle$$

This is just like, for example, the fact that we can expand the spin state of the electron either in the z-spin or x-spin bases.

$$|\psi\rangle \;=\; \alpha\,|\uparrow\rangle + \beta\,|\downarrow\rangle \qquad \text{or} \qquad |\psi\rangle \;=\; \gamma\,|\rightarrow\rangle + \delta\,|\leftarrow\rangle$$

Fourier transforms

- $\psi(x)$ and $\tilde{\psi}(k)$ are Fourier transforms of one another.

$$\tilde{\psi}(k) \;=\; \langle k \,|\, \psi \,\rangle \;=\; \int \langle k \,|\, x' \,\rangle \,\langle x' \,|\, \psi \,\rangle \, dx' \;=\; \frac{1}{\sqrt{2\pi}} \int e^{-ikx'} \psi(x') \, dx'$$

Similarly, using $\int |k'\rangle\langle k'| \, dk' \;=\; \hat{I}$ we have:

$$\psi(x) \;=\; \langle x \,|\, \psi \,\rangle \;=\; \int \langle x \,|\, k' \,\rangle \,\langle k' \,|\, \psi \,\rangle \, dk' \;=\; \frac{1}{\sqrt{2\pi}} \int e^{ik'x} \tilde{\psi}(k') \, dk'$$

The momentum operator, $\hat{p}$

- Since $\hat{k}$ is a Hermitian operator, it corresponds to an observable. The observable corresponding to $\hat{k}$ is $p/\hbar$, the momentum divided by $\hbar$. We can define then the momentum operator as: $\hat{p} \;=\; \hbar\hat{k}$. You will have to just accept this for now. We'll see later that the expectation value of $\hat{p}$ corresponds to momentum in the classical limit.

- Substituting $\hbar p$ for k, we have:

$$\tilde{\psi}(p) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int e^{-ipx'/\hbar} \, \psi(x') \, dx' \qquad\qquad \psi(x) \;=\; \frac{1}{\sqrt{2\pi\hbar}} \int e^{ip'x/\hbar} \, \tilde{\psi}(p') \, dp'$$

- The state of a particle is given by either specifying $\psi(x)$ or $\tilde{\psi}(p)$ but not both. Specifying one completely determines the other through the Fourier transform. Note that this is very different from classical physics where the state of a particle is specified by giving its position, x, <u>and</u> its momentum, p.

Correspondences between the x and k (or p) representations

- There is a symmetry between the x and k representations and a one-to-one correspondence between an expression in the x representation and a corresponding expression in the k representation. The table on the following page, illustrates this.

x-representation	k-representation
eigenstates: $\|x\rangle$	eigenstates: $\|k\rangle$
$\langle x \,\|\, \psi \rangle = \psi(x)$	$\langle k \,\|\, \psi \rangle = \tilde{\psi}(k)$
$\|\psi\rangle = \int \psi(x')\,\|x'\rangle\,dx'$	$\|\psi\rangle = \int \tilde{\psi}(k')\,\|k'\rangle\,dk'$
$\int \|x'\rangle\langle x'\|\,dx' = \hat{I}$	$\int \|k'\rangle\langle k'\|\,dk' = \hat{I}$
$\langle \psi \,\|\, \psi \rangle = \int \psi^*(x')\psi(x')\,dx'$	$\langle \psi \,\|\, \psi \rangle = \int \tilde{\psi}^*(k')\tilde{\psi}(k')\,dk'$
$\langle x\|\hat{x}\,\|\psi\rangle = x\,\psi(x)$	$\langle k\|\hat{x}\,\|\psi\rangle = i\,\frac{d}{dk}\,\tilde{\psi}(k)$
$\langle x\|\hat{k}\,\|\psi\rangle = -i\,\frac{d}{dx}\,\psi(x)$	$\langle k\|\hat{k}\,\|\psi\rangle = k\,\tilde{\psi}(k)$
$\langle x \,\|\, x_0 \rangle = \delta(x - x_0)$	$\langle k \,\|\, x_0 \rangle = \frac{1}{\sqrt{2\pi}}\,e^{-ikx_0}$
$\langle x \,\|\, k_0 \rangle = \frac{1}{\sqrt{2\pi}}\,e^{ik_0x}$	$\langle k \,\|\, k_0 \rangle = \delta(k - k_0)$
$\langle x \,\|\, p_0 \rangle = \frac{1}{\sqrt{2\pi\hbar}}\,e^{ik_0x/\hbar}$	$\langle p \,\|\, x_0 \rangle = \frac{1}{\sqrt{2\pi\hbar}}\,e^{-ipx_0/\hbar}$

Are position and momentum really continuous?

- If space is continuous, then states of definite position are represented in the position basis as δ-functions.

$$\psi_{x_0}(x) = \langle x \,|\, x_0 \rangle = \int_{-\infty}^{\infty} \langle x \,|\, k' \rangle \langle k' \,|\, x_0 \rangle \, dk'$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik'(x-x_0)}\, dk' = \delta(x - x_0)$$

Notice that $\psi_{x_0}(x)$ is a $\delta(x - x_0)$ only if the limits of integration are $\pm\infty$. If the limits of integration are $\pm K$, we then have:

$$\frac{1}{2\pi} \int_{-K}^{K} e^{ik'(x-x_0)}\, dk' = \frac{1}{\pi} \frac{\sin K(x - x_0)}{x - x_0}$$

This has a width of π/K.

- A continuous spectrum of position states requires that k and therefore the momentum range from $-\infty$ to $+\infty$. Since there is not an infinite amount of energy in the universe, the momentum can only range between finite limits $\pm P = \pm\hbar K$. The position is then quantized in steps of $\pi n\hbar/P$ where n is an integer.

- Similarly, if k is continuous, states of definite k are represented in the k basis as δ-functions.

$$\tilde{\psi}_{k_0}(p) = \langle k \,|\, k_0 \rangle = \int_{-\infty}^{\infty} \langle p \,|\, x' \rangle \langle x' \,|\, k_0 \rangle \, dx'$$

$$= \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{-i(k-k_0)x'} \, dx' = \delta(k - k_0)$$

- A continuous spectrum of momentum states requires that x range from $-\infty$ to $+\infty$. Since the universe is not infinitely large, the space can only range between finite limits $\pm L$. Momentum is then quantized in steps of $\pi n\hbar/L$ where n is an integer.

- We previously saw that continuous position and continuous momentum distributions lead to the problem of δ-function normalization of the respective eigenstates. We now see that since the universe has neither an infinite amount of energy nor an infinite extent, the distributions in position and in momentum are not really continuous. However, since it's much easy to do integrate than to sum over a huge numbers of terms, we pretend that space and momentum are effectively continuous.